

ECOSAR Computer Program

Abstract

OPPT uses Structure Activity Relationships (SAR) to predict the environmental toxicity of chemicals to aquatic organisms. To share the methodology with the chemical industry and others, OPPT has developed a software program called ECOSAR and its user's manual, which are regularly updated.

ECOSAR predicts acute and chronic toxicity of industrial chemicals to aquatic organisms without the need to perform actual toxicity tests. The software program called ECOSAR depends on the principle that there are predictable relationships between a chemical's structure and physical/chemical properties on one hand, and its toxicity or biological activity on the other hand. If researchers know the toxicity of one or more chemicals in a class or category of chemicals, SARs can be used to predict the toxicity of other chemicals in that class or category. The chemical industry and others can use ECOSAR (1) to predict the toxicity profile of new chemicals prior to PMN submission, (2) to predict the toxicity of a chemical prior to actual toxicity testing, (3) to judge the validity of actual toxicity testing for a chemical, (4) to fill data gaps in a chemical's toxicity profile, and (5) to screen for environmental toxicity when seeking safer substitutes for existing or new chemicals.

OPPT has produced a new version of ECOSAR which is a significant improvement over the original version published in 1994. In order to use the original version of ECOSAR a user has to have a working knowledge of organic chemistry and the SARs used by OPPT. The new version of ECOSAR has a new subroutine which does not require the user to have an extensive knowledge of organic chemistry or the types of SARs used by OPPT. The user simply has to input the chemical's structure or its Chemical Abstract Service Registry Number (CASRN). The new subroutine analyzes the chemical structure and automatically selects the SARs that OPPT would use in assessing the chemical. A toxicity profile for the chemical is automatically printed. In addition, the new version of ECOSAR has new SARs, updated SARs, and can be used in a WINDOWS configuration. ECOSAR and its user's manual may be obtained from EPA at <http://www.epa.gov/opptintr/newchms/>. Click on the ECOSAR button bar. Directions for downloading are on the second page of the fact sheet. New versions are added as they become available. Enjoy. For questions: contact J. Vincent Nabholz at 202.260.1271 or nabholz.joe@epa.gov.

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Education

Ph.D. from the University of Georgia, Athens in 1978.

His duties with OPPT have included the pragmatic application of the theory of chemical structure activity relationships for the routine risk assessment of industrial chemicals under TSCA, the development of protocols/guidelines for testing chemicals for toxicity, and the validation of toxicity test results.